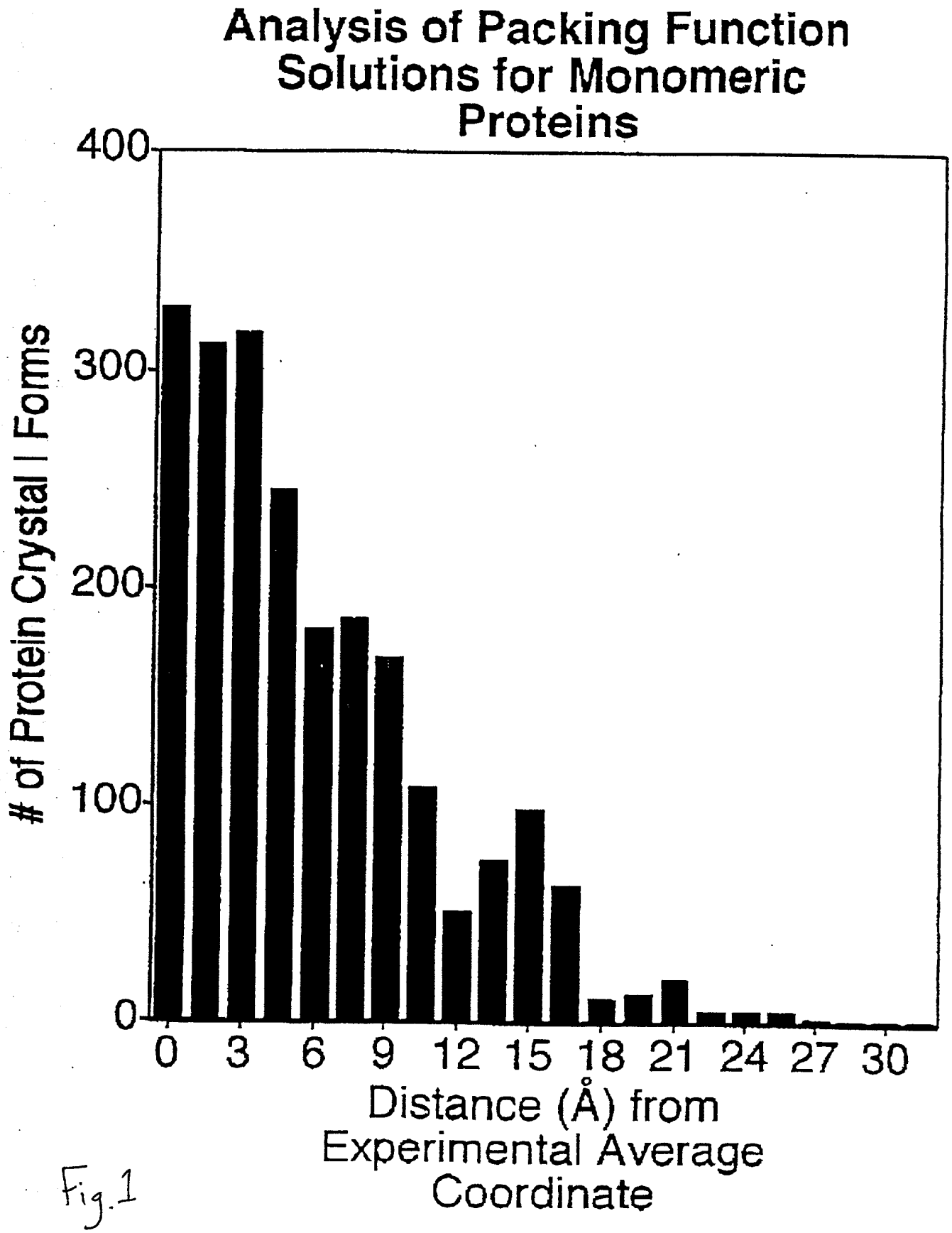

Analysis of Packing Function Solutions for Monomeric Proteins
# of Protein Crystal I Forms
400
300
200
100
0
0 3 6 9 12 15 18 21 24 27 30
Distance (Å) from Experimental Average Coordinate

Fig. 1

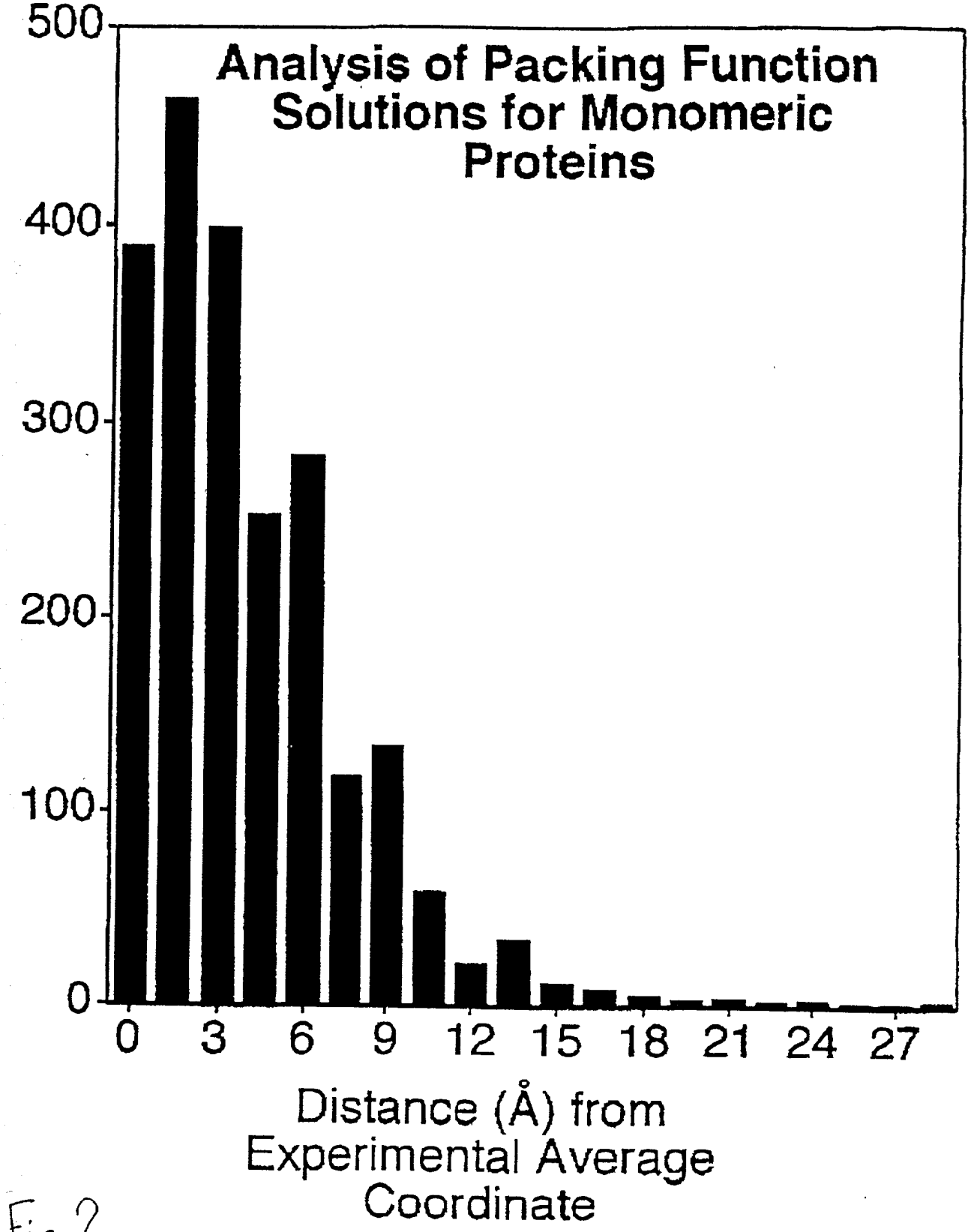

Analysis of Packing Function Solutions for Monomeric Proteins
# of Protein Crystal Foms
500
400
300
200
100
0
0 3 6 9 12 15 18 21 24 27
Distance (Å) from Experimental Average Coordinate

Fig. 2

START:

Set Up Parallelization

Initialize Constants and Sine/Cosine Tables

Input 1 & Initialize the List of Fourier Indices (hkl)

Get Biggest Sphere Without Overlap of Symmetry Mates

Input 2

Confirm Calculation Mode

Initialize Tables of Spherical Bessel Functions and Bessel Function 0's

Determine Limits on l & m indices and on n indices at each l

For modes 5 thru 7: Read expected SHSB coefficient & deviation values

For Use with a Radial Correction or with Modes 5 thru 7:

Get Fractionalization Matrix

Partition the List of Fourier Indices Between Processor(s)

Convert Each Fourier Index (hkl) to Polar Coordinates & Get Its Bessel Argument

Get the FT of a Crystalline Unit Cell Filled with Symmetry Related Spheres

Calculate a Radial Correction Factor for Each "n" Index

Calculation Mode-Specific Routines:

Modes 1 & 2 (Unphased Diffraction Amplitudes to Phased FT of SHSB-modeled Unit Cell)

Mode-Specific Input

Get Input File # for Calculated FT, if there is a Prior Model

Initialize Correlation Exponentiation Factor

Modes 1& 2 (cont'd)

Cycle For Each Choice (mstop) of Stopping Value for the SHSB m index

Update Correlation Exponentiation Factor

If there is a Prior Model (On cycles after the 1st cycle of the 1st run of the program):

On Cycles After the 1st value of mstop Update the File # for the Calculated FT

For Each input SHSB Model

Convert the File # & the Model # to a File Name

Read Input FT & SHSB coefs of the Prior Model

If there is No Prior Model:

Model the Crystal as a Crystalline Unit Cell Filled with Symmetry Related Spheres

Get a Starting Value (msus) for the SHSB m Index for the Next Packet of m Values

Update the Model by Adjusting the Contributions of each SHSB function for each lmn index in the m-packet from 'msus' to 'mstop'

Fig. 3

Flow Chart for the Main Driver Program for "faizer": Options to compute a the FT of a SHSB Model of Crystal

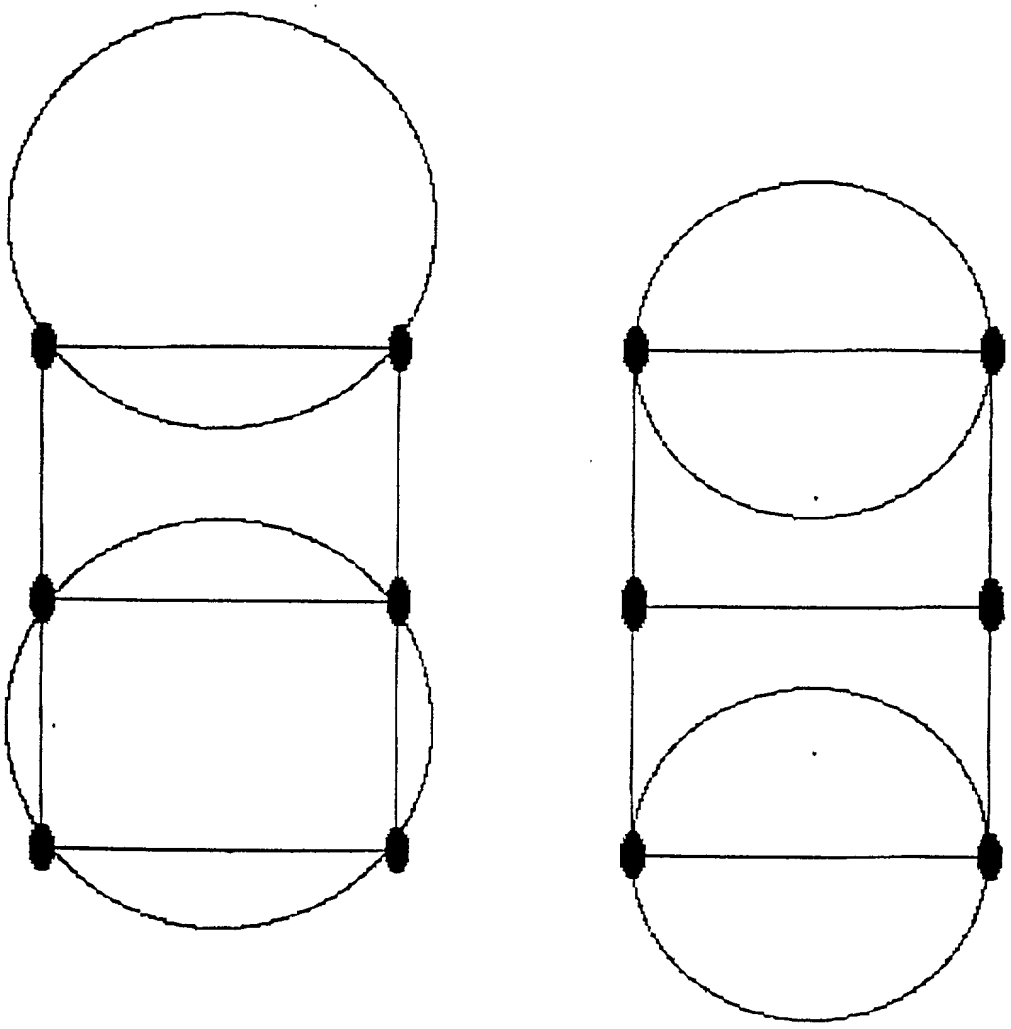


Figure 4 A schematic example: Two choices for filling the same portion of a crystal unit cell from an orthorhombic Spacegroup. Although the spheres on the right are smaller than those on the left, for some crystals, the local maximum in the packing on the right wold be the packing of maximal consistency with the crystallographic data.

Figure 4.

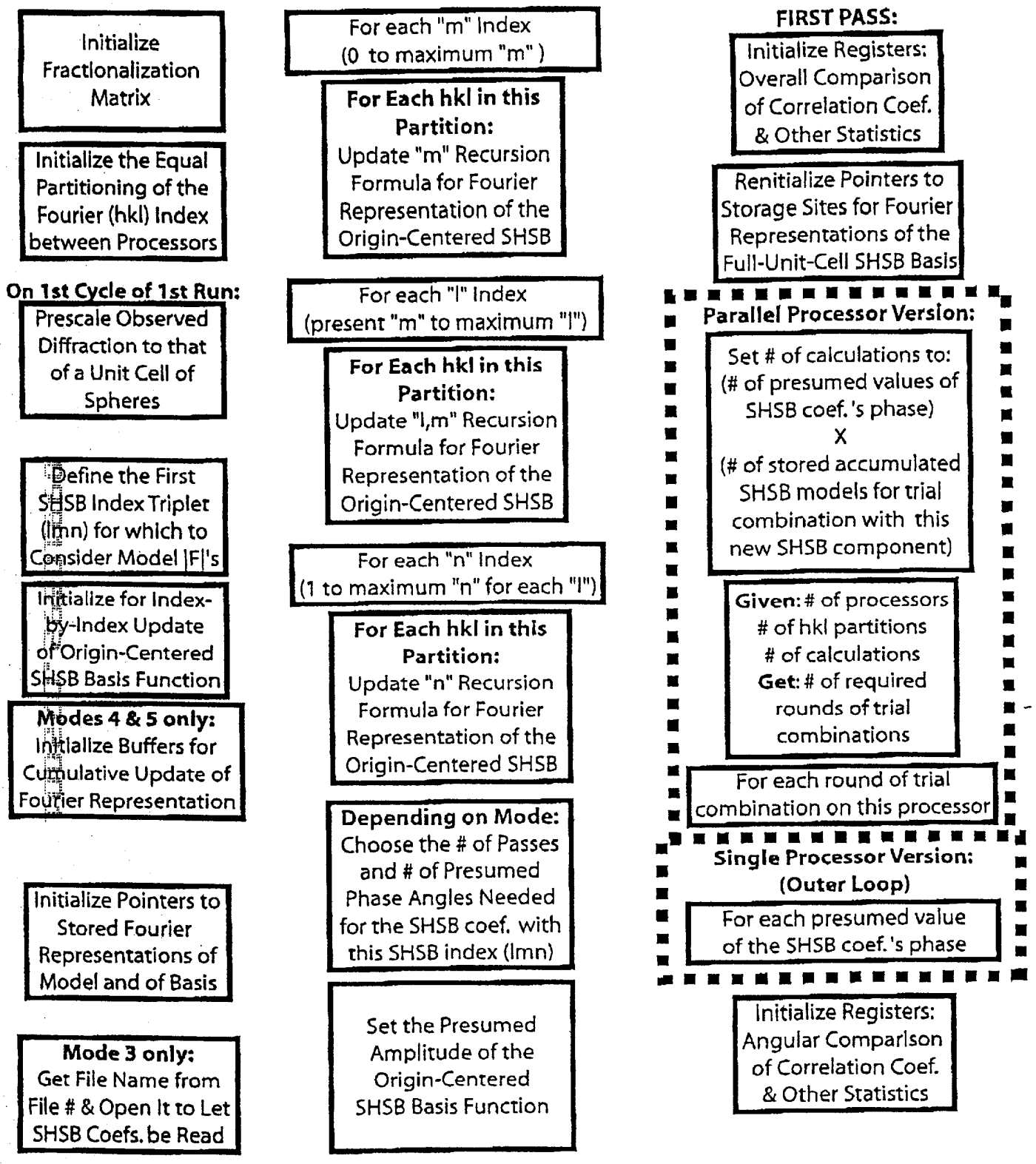
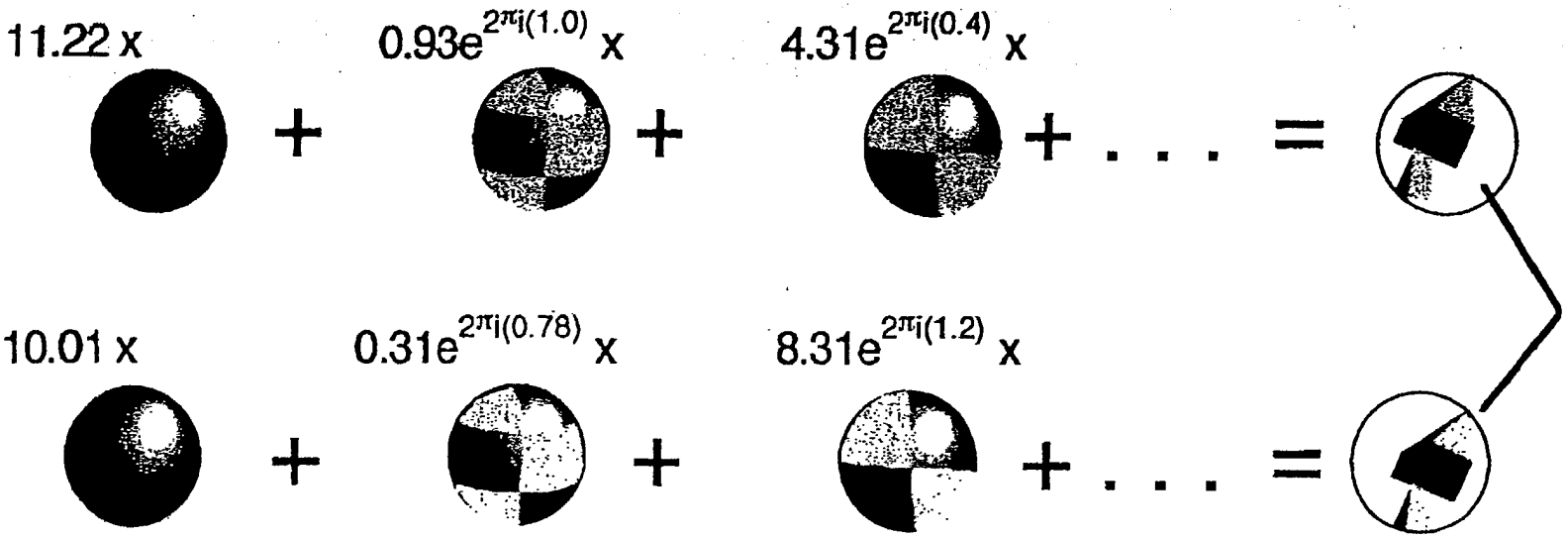

Initialize Fractionalization Matrix
Initialize the Equal Partitioning of the Fourier (hkl) Index between Processors
On 1st Cycle of 1st Run:
Prescale Observed Diffraction to that of a Unit Cell of Spheres
Define the First SHSB Index Triplet (lmn) for which to Consider Model |F|'s
Initialize for Index-by-Index Update of Origin-Centered SHSB Basis Function
Modes 4 & 5 only:
Initialize Buffers for Cumulative Update of Fourier Representation
Initialize Pointers to Stored Fourier Representations of Model and of Basis
Mode 3 only:
Get File Name from File # & Open It to Let SHSB Coefs. be Read
For each "m" Index
(0 to maximum "m")
For Each hkl in this Partition:
Update "m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB
For each "l" Index
(present "m" to maximum "l")
For Each hkl in this Partition:
Update "l,m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB
For each "n" Index
(1 to maximum "n" for each "l")
For Each hkl in this Partition:
Update "n" Recursion Formula for Fourier Representation of the Origin-Centered SHSB
Depending on Mode:
Choose the # of Passes and # of Presumed Phase Angles Needed for the SHSB coef. with this SHSB index (lmn)
Set the Presumed Amplitude of the Origin-Centered SHSB Basis Function
FIRST PASS:
Initialize Registers: Overall Comparison of Correlation Coef. & Other Statistics
Renitialize Pointers to Storage Sites for Fourier Representations of the Full-Unit-Cell SHSB Basis
Parallel Processor Version:
Set # of calculations to:
(# of presumed values of SHSB coef.'s phase)
X
(# of stored accumulated SHSB models for trial combination with this new SHSB component)
Given: # of processors
# of hkl partitions
# of calculations
Get: # of required rounds of trial combinations
For each round of trial combination on this processor
Single Processor Version:
(Outer Loop)
For each presumed value of the SHSB coef.'s phase
Initialize Registers: Angular Comparison of Correlation Coef. & Other Statistics

Fig. 5

Identical Image from Expansions about Different Origins:



Symmetry Expanded Direct Space Basis Functions:

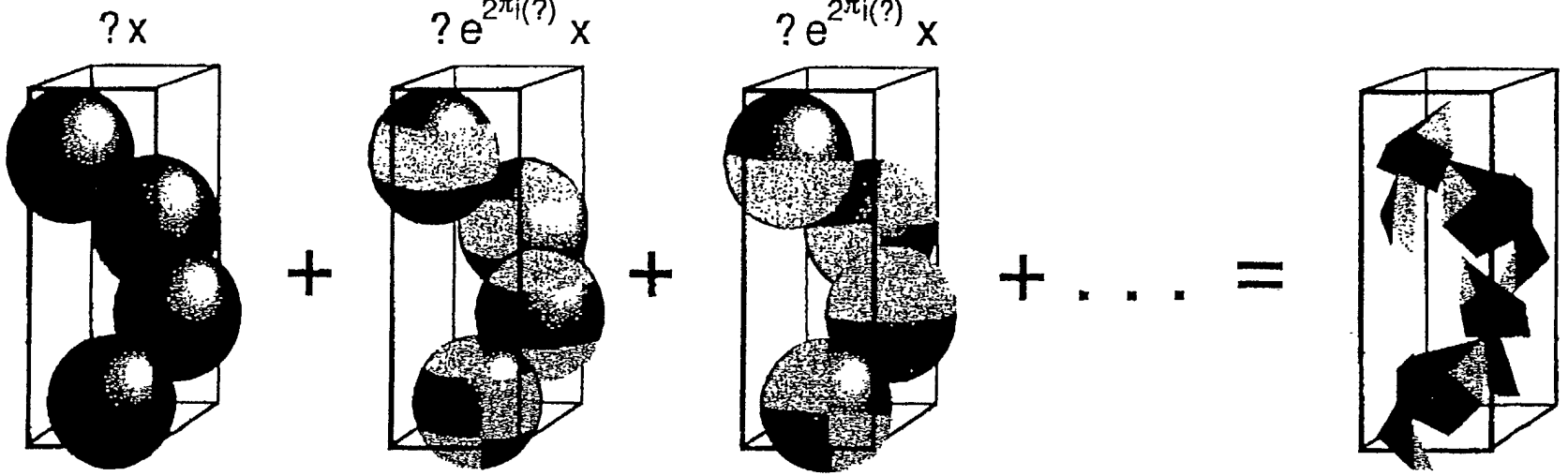
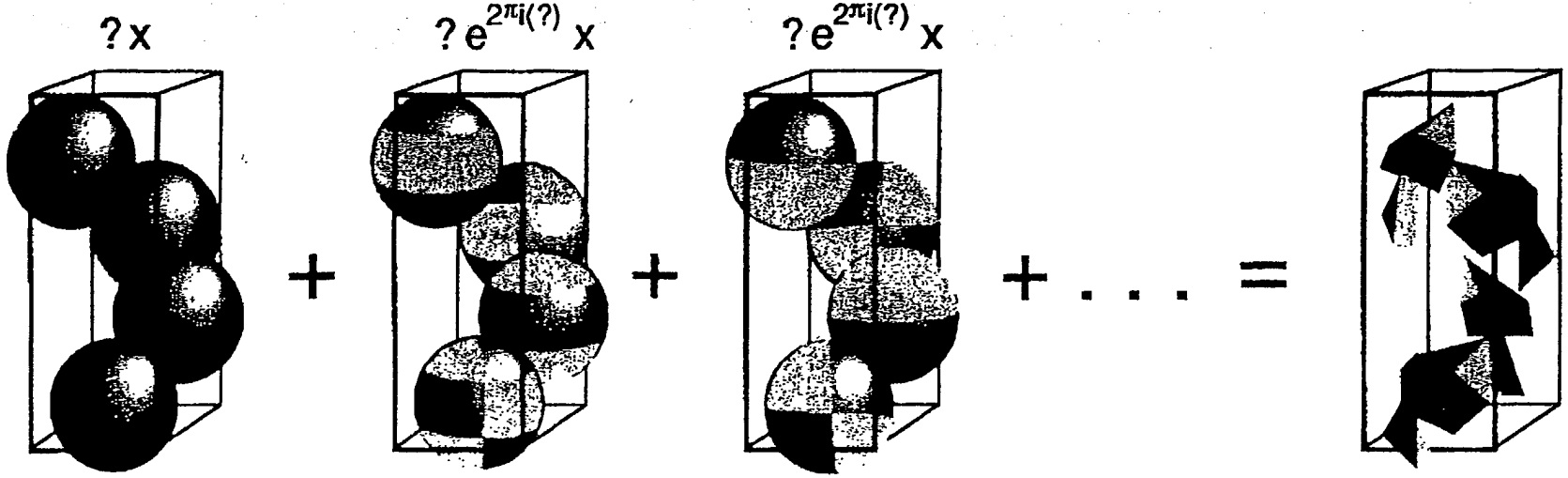


Fig. 6

With a properly chosen origin, 45-55% of the unit cell can be expanded. (Most protein crystals are > 45% solvent.)

Component Direct Space Basis Functions:



Component Fourier Transforms:

$$a_{001}F_{solo}^{001}(hkl) + a_{211}F_{solo}^{211}(hkl) + a_{111}F_{solo}^{111}(hkl) + \ldots = F_{obs}(hkl)$$

$$a_{001} = \Sigma_{hkl} F^{*}_{solo}{}^{001}(hkl)\, F_{obs}(hkl) \quad [\text{presume } \phi = 0.00 \text{ to start}]$$

$$F_{accum}(hkl) = a_{001}F_{solo}^{001}(hkl)$$

$$a_{211} = \Sigma_{hkl} F^{*}_{solo}{}^{211}(hkl)\, (|F_{obs}(hkl)| - |F^{n}_{accum}(hkl)|)e^{2\pi i \phi^{n}_{accum}(hkl)}$$

$$F^{n+1}_{accum}(hkl) = F^{n}_{accum}(hkl) + a_{211}F_{solo}^{211}(hkl)$$

Fig. 7